## Executive Summary

This work was aimed at developing and applying a new methodology for the efficient and accurate computation of problems involving several phases of matter. In particular, solidification processes typically involve melt/solid and sometimes melt//gas interfaces, whose location and shape is unknown a priori. This class of problems is called free or moving boundary problem, and the numerical approaches for its solution to date are inaccurate, inefficient, and can not be readily extended to multi-dimensions or to time dependent phenomenon.

Ongoing research on welding at ONR and on crystal growth at NASA and other institutions all fall into the category of free boundary problems. It is exactly the accurate determination of the process dynamics and the shape and location of the interface between the phases which is responsible for the ultimate chemical segregation and the mechanical properties in the solid.

This work developed the Triad Field Formalism approach for the computation of general multi-dimensional and time dependent free boundary problems. The particular subject addressed is solidification phenomena. All the relevant boundary conditions on the developing interface were exactly resolved. Several computer programs were developed during the course of this research, enabling us to determine for the first time the interplay among the various fields operating in tandem to produce the phenomena observed during solidification processes in weld pools and during crystal growth.

# Time-dependent Numerical Simulations of Solidification Processes

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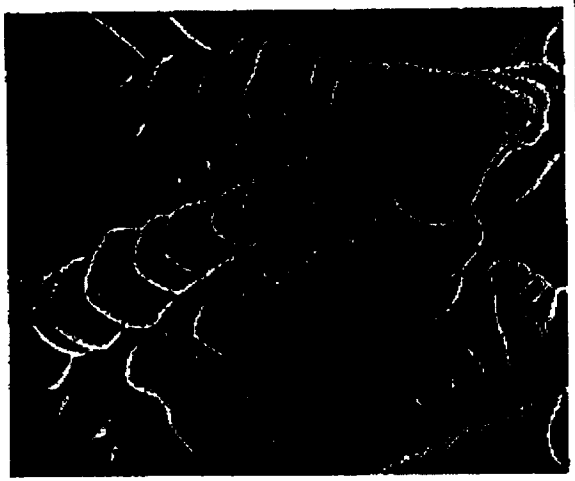
(NASA / ONR co-funded)

Dendrites form the most ubiquitous of solidification microstructures. Accurate prediction of their size and solidification rates are critical to design, prediction, and analysis of materials properties.



## Objectives:

- Develop accurate theoretical and numerical tools to predict dendritic microstructure formation.
- Demonstrate and apply tools to benchmark experiments and to industrial and other Navy projects.

## Approach:

- Develop accurate physical and mathematical description of dendritic formation.
- Develop novel numerical techniques for analyzing solidification phenomena using a new multi-dimensional, time-dependent free-surface algorithm.

## Payoff:

- First general predictive theory for dendritic growth verified by benchmark experiments.
- Ability to predict cellular and dendritic microstructure using numerical simulations.
- Future impact on analysis and control of microstructure development during critical processes such as casting and welding.

Text of Report

The phenomenon of a phase change is among the distinguishing features of most materials processes. This phenomenon belongs to a class of problems governed by the existence of a free boundary, or an interface, between phases. This interface may be geometrically simple to describe, but more often than not, a very complex one. The problem of the phase-change interface instability which leads to the commonly observed interface morphologies has proven to be extremely difficult to solve, despite the substantial attention devoted to it over the past several decades. The physical processes involve a delicate balance among several parameters, including surface tension, anisotropy, latent heat requirements and kinetic and concentration effects, all operating on the heat and mass transfer fields determined by both diffusion and convection. The surface instabilities result in an extremely rich set of interfacial phenomena, including cells and dendrites, among others. The mathematical treatment of this problem is presently a hotly-debated issue in the literature.

A new numerical algorithm for the computation of free-boundary problems has been developed. The algorithm, called the Triad Field Algorithm, borrows concepts from advanced mathematical treatment of similar problems in astrophysics, and is a generalization of the powerful computational technique of numerical grid generation. The formulation is based upon a time dependent mapping technique enabling the resolution of complex multi-dimensional geometries and boundary conditions. The mapping essentially immobilizes the domain, resulting in a solution of a more complicated set of equations, but on a time independent regular domain (usually a rectangular or cubic geometry). The equations on the transformed domain can be solved using a variety of efficient

numerical techniques suitable for regular domains which could be readily adopted to vector and parallel computers. In this study we developed a multi-dimensional time dependent formulation of the Triad Field Algorithm. We initially studied several fundamental problems in phase transition using the numerical adaptation of the algorithm. In particular, the development of interfacial features such as cells and dendrites during solidification, together with the evolution of the microscgregation in the solidifying portion, were examined without ad-hoc assumptions.

This study is of significant fundamental and applied value. The problem of non-linear pattern formation has attracted great interest in the past several years, but most approaches to-date involved severe simplification resulting in solution of model mathematical equations which often possess little physical meaning. The approach in this work starts from the governing physical equations and avoids any simplifications. The applied significance of this work can be readily understood since the resulting interfacial patterns are responsible for the development of the microsegregation and hence the final mechanical properties of most solid components produced today.

This work is also of direct relevance to modeling of solidification research in welding and crystal growth processes. These processes are typically characterized by extremely complex fluid, heat. and mass transport driven by strong thermal and solutal gradients, all operating with commonly two unstable free surfaces, gas/melt and solid/melt. Despite significant advances in the area of Computational Fluid Dynamics (CFD), techniques to compute these unstable free boundary problems in multi-dimensions are inexact and poorly model the correct physical phenomena on these boundary. However, it is precisely those boundary conditions which determine the fields in the melt, and the chemical segregation and the

thermal stresses in the solid.

This work complemented both NASA and ONR, and other on-going traditional research in this area by building an alternative computational framework which can be readily extended in the future to systematically add additional physical phenomena in the process.

The work on formulating and applying the Triad Fieid Formalism method to deeply nonlinear stages of solidification fronts was carried out. We have demonstrated the importance of the time dependent aspects of the problem as crucial for the natural development of cellular and predendritic microstructures from arbitrary initial conditions. This finding, reported in the literature in two publications and in an international conference, is in direct conflict with presently postulated theories which are based on steady-state models. The major problems in such model is the need for additional parameters for existence of physically accepted solutions to the steady-state problem. We have directly demonstrated that these results are an artifact of the mathematical simplification made a priori in the model development. We presented physically realizable solutions without resorting to such simplifications.

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Time dependent theory and numerical simulation of the morphological instability during solidification were developed and verified. Both new theories and numerical codes were developed and applied to a variety of unstable morpologics. Novel results, confirmed by experiments, were obtained for dendritic solidification.

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